

Von Neumann Turbulent Transport Model

J. I. Katz

Department of Physics and McDonnell Center for the Space Sciences

*Washington University, St. Louis, Mo. 63130**

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Abstract

I propose a simple model, based on an analogy to von Neumann artificial viscosity, of turbulent diffusion, heat diffusion and viscosity coefficients for use in modeling subgrid turbulent diffusivity in multi-phase numerical hydrodynamics and, more generally, in subgrid turbulent viscosity and thermal transport. In analogy to the von Neumann artificial viscosity, these coefficients explicitly contain the grid size and do not attempt a quantitative model of the unresolved turbulence. In order to address the problem that it is often not known *a priori* when and where a flow will become turbulent, the coefficients are set to zero when the flow is not expected to be turbulent on the basis of a Richardson/Rayleigh-Taylor stability criterion, in analogy to von Neumann's setting of artificial viscosity to zero in expanding flows.

Keywords: numerical methods, transport coefficients, diffusion, viscosity

*Electronic address: katz@wuphys.wustl.edu

I. INTRODUCTION

Turbulent diffusion in heterogeneous or multi-phase flows and turbulent viscosity and heat transport in all flows are problems of great practical importance in numerical hydrodynamics. In many problems the Reynolds number is enormous and if the flow becomes turbulent it is not possible to calculate it explicitly on the finer scales of heterogeneity that are still large enough that microscopic transport processes (diffusivity, viscosity and conductivity) have not smoothed out the variations in the corresponding physical variables.

When the composition of the fluid is heterogeneous the most important questions usually concern the mixing of material of different compositions or in different phases [1], rather than the turbulent momentum transfer. A number of sophisticated turbulence models have been developed, including the “K-L” model [2] of Rayleigh-Taylor and Richtmyer-Meshkov instability and the more general BHRZ model [3] (sometimes called the BHR model) that implicitly account for all sources driving instability and turbulence, including shear (Kelvin-Helmholtz instability), through their derivation from the Euler equations. As powerful as these models are, they can be complex to implement because they describe the strength of turbulence with parameters that are non-local and history-dependent functions of space and time. The success of the very simple von Neumann [4] artificial viscosity, nearly universally used in numerical calculations of compressible flow, suggests that a similarly simple model of turbulent transport, may be useful.

II. GENERAL CONSIDERATIONS

The elementary Kolmogorov turbulence model indicates an eddy turnover time

$$t_k \propto k^{-2/3}, \quad (1)$$

for eddy size $1/k$. Hence if the flow is turbulent at all small eddies turn over much faster than larger ones. Assuming at least one turnover for the largest driving eddies there is likely to be rapid mixing down to the inner turbulence scale.

If the Schmidt number

$$\text{Sc} \equiv \frac{\nu}{D}, \quad (2)$$

where ν is the kinematic viscosity and D the diffusivity, is of order unity or less then diffusive mixing on scales smaller than the inner turbulence scale will be at least as rapid as the

turnover of the smallest eddies, and much more rapid than that of the driving eddies. This is usually the case because in dilute gases or weakly coupled liquids momentum, thermal energy and composition are, to a substantial extent, carried by the same particles (in a plasma momentum is almost entirely carried by the ions and energy by the electrons; at sufficiently high Reynolds number all of these quantities diffuse on the inner turbulence scale much faster than the turnover of the driving eddies). Only if $Sc \gg 1$ may diffusion down to the molecular or atomic scale be slower than turbulent turnover; this may occur when the viscosity is large because of strong intermolecular forces, as in viscous liquids (glycerin, honey, pitch, the Earth's mantle, *etc.*) in which momentum diffuses rapidly but chemical composition slowly. Such substances rarely undergo turbulent high Reynolds number flows, though such flows are, in principle, possible if driven strongly enough.

In the classical Kolmogorov turbulent cascade the inner scale ℓ_{in} of turbulence is approximated by

$$\ell_{in} \approx \left(\frac{\nu^3}{\epsilon} \right)^{1/4}, \quad (3)$$

where ν is the kinematic viscosity and $\epsilon \sim U^3/R$ is the kinematic (per unit density) energy dissipation per unit volume of a flow with characteristic velocity U on an outer scale R . This leads to an estimate of the time for microscopic diffusion to produce atomic-scale homogeneity

$$t_{diff} \approx \frac{\ell_{in}^2}{D} \approx Sc \sqrt{\frac{\nu R}{U^3}} \approx \frac{Sc}{\sqrt{Re}} t_{turn}, \quad (4)$$

where the turnover time $t_{turn} \equiv R/U$. In high Reynolds number flows microscopic (diffusive) mixing on length scales from ℓ_{in} down to atomic dimensions is a very rapid process unless the $Sc \gg 1$.

Turbulent heat transport presents similar problems. If the Prandtl number

$$Pr \equiv \frac{\nu}{\alpha}, \quad (5)$$

where α is the microscopic heat diffusion coefficient, is of order unity or less then diffusive heat transfer on scales smaller than the inner turbulence scale will be at least as rapid as the turnover of the smallest eddies, and much more rapid than that of the driving eddies. This is usually the case because in dilute gases or weakly coupled liquids momentum and thermal energy are, to a substantial extent, carried by the same particles. In liquid metals or ionized plasmas the rapid thermal conduction by electrons or rapid radiative transfer lead to $Pr \ll 1$

and this inequality holds even more strongly. Just as for turbulent mixing, only in viscous liquids in which strong intermolecular forces carry momentum is $\text{Pr} \gg 1$ and the efficacy of diffusive heat transport on scales smaller than the inner turbulence scale is problematic; this paper does not discuss that regime.

III. TURBULENCE CRITERION

The problem is to model the subgrid diffusion in fluids with $\text{Sc} \lesssim 1$ when small features of the flow cannot feasibly be resolved computationally. This requires a criterion to decide when the flow is turbulent as well as a model for turbulent mix. It is often not possible to perform an instability analysis because of the complexity and non-stationary character of the large scale flow in problems such as inertial confinement fusion. The recognition that a complex flow is turbulent and will possess a turbulent cascade to large wave numbers, much less the determination of its characteristics, is non-trivial. This limits the usefulness of even the most sophisticated turbulence models.

Because microscopic diffusion on scales smaller than ℓ_{in} is generally much faster than the lifetime of the flow, which is generally $\mathcal{O}(t_{turn})$, determining whether a flow is turbulent on scales $\sim \ell_{in}$ not explicitly resolved in a numerical calculation is much more important than a quantitative estimate of the turbulent diffusion coefficient itself. A common criterion for whether a computed or observed flow is turbulent is “I know it when I see it”. This is useless in a large numerical simulation in which the structure of the flow is not known in advance. A simple and automatic turbulence criterion is required. Without knowing if a flow is turbulent or not it is impossible even to decide if a turbulence model should be used at all, much less to make reasonable estimates of its parameters.

The model presented here is almost childishly naïve compared to the non-oscillatory finite volume (NFV) difference schemes[5, 6] that have been remarkably successful in modeling turbulent flows. So is the von Neumann artificial viscosity, yet it remains the basis of most numerical calculations of compressible flows.

The present model uses an on-off switch on turbulent transport based on the Richardson stability criterion appropriate to high Reynolds number shear flow (if there is no shear it reverts to the Rayleigh-Taylor stability criterion for inviscid miscible fluids). This switch is a generalization of one used ([2]) in the “K-L” model of turbulence produced by Rayleigh-

Taylor and Richtmyer-Meshkov instability. An implicit switch is present in the more general BHRZ model [3] of turbulence in which the explicitly calculated velocity field drives or damps turbulence according to the Euler equations.

A switch is not needed in calculations of flows (such as unstratified pipe flows) that are known *a priori* to be unstable, and that constitute the usual tests of turbulence models. It is essential in more complex heterogeneous flows that contain both stable and unstable regions that are not predictable in advance. The switch is analogous to the switch in the von Neumann artificial viscosity that sets it to zero in rarefying regions.

Sub grid scale (SGS) turbulence models of this type were first proposed by Smagorinsky [7] for use in numerical large-eddy simulations (LES) of flows whose small scale turbulence is numerically unresolved. Many SGS models have been developed since his pioneering work [8, 9, 10, 11], but none appear to be universally applicable. In this paper I follow von Neumann’s [4] artificial viscosity model for dissipation in unresolved shocks, by renouncing any attempt to model the SGS turbulence in detail or on the basis of fundamental principles, just as [4] renounced any attempt to understand the microscopic dissipation mechanisms and structure of shocks (which also depend on the detailed physics of the particular fluids involved, so that no single model can be generally valid), and construct a model that instead depends explicitly on the numerical properties of the LES, while incorporating a criterion for instability and the *presence* of turbulence and turbulent diffusivity that explicitly depends on the resolved properties of the flow.

IV. MODEL TURBULENT DIFFUSIVITY

This problem has some similarity to that of modeling shocks in compressible flow. In each problem the difficulty is posed by subgrid scale dissipative processes that cannot be resolved computationally, but are known to be present. The classic solution[4] is to define an “artificial viscosity” that is explicitly dependent on the grid size (thus broadening a shock to a width of a few resolution elements) and introducing a nonlinear criterion for its presence, in essence an on-off switch that turns it on when the fluid is being compressed and off when being rarefied (because in thermodynamically stable systems there are no rarefaction shocks). The resulting artificial viscosity is strongly nonlinear and has the unphysical property of a magnitude that depends on the scale of the computational grid. It has been widely adopted because

it accurately reproduces the shock jump conditions, at the price of not reproducing the structure of the shock on the scale of the grid resolution or its (much finer and unresolvable) actual microscopic structure. It has the same dimensions as real physical viscosity.

We seek an analogous heuristic artificial diffusivity for multicomponent flows. The turbulent diffusivity we propose is

$$D_{turb} = \begin{cases} 0 & \text{if } \frac{\vec{a} \cdot \nabla \rho'}{\rho' |e_{ij}|^2} \geq \frac{1}{4}, \\ \frac{\Delta^2 |e_{ij}|}{6} & \text{if } \frac{\vec{a} \cdot \nabla \rho'}{\rho' |e_{ij}|^2} < \frac{1}{4}; \end{cases} \quad (6)$$

where \vec{a} is the local fluid acceleration, Δ is a characteristic (filter) length,

$$e_{ij} \equiv \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}, \quad (7)$$

is the traceless (anisotropic) symmetrized strain rate tensor [12, 13] and

$$|e_{ij}| = \sqrt{e_{ij} e_{ij}} \quad (8)$$

is its scalar magnitude; summation over repeated indices is implicit. This D_{turb} is analogous to the Smagorinsky turbulent viscosity model of subscale eddy simulation (see [14] for a review).

A number of heuristic prescriptions for Δ have been used [15, 16, 17]. Without an opportunity to compare to detailed experimental data in complex and difficult to diagnose flows such as those encountered in inertial confinement fusion, it is hard to decide which is most appropriate for those flows, and the best prescription may vary over space and time. We suggest that Δ be taken to be the smallest dimension of a spatial zone because high aspect ratio zones are generally used only when there are large gradients of composition or other variables in the direction of the smallest side of a zone that need to be resolved; these smallest sides are likely to limit mixing lengths.

Alternative forms are possible. For example, a tensor D_{ij} could be defined by replacing $|e_{ij}|$ by e_{ij} in the expression for D_{turb} . However, if the turbulent cascade isotropizes the turbulence, as generally assumed in the absence of a quantitative more general model, then the subgrid D_{turb} should be a scalar, as in the form above.

The on-off switch is adapted from the Richardson instability criterion [18, 19] in stratified fluids, replacing the stratifying acceleration of gravity \vec{g} by the component of local acceleration \vec{a} along the gradient of potential density:

$$\nabla \rho' \equiv \nabla \rho - \frac{\partial \rho}{\partial p} \bigg| \nabla p, \quad (9)$$

where the partial derivative is evaluated under thermodynamic conditions appropriate to matter displacements. If flows are nearly adiabatic on displacement time scales this is $\frac{\partial \rho}{\partial p}\big|_S$, while if they are nearly isothermal (as will be the case if conductive or radiative energy transfer to a heat bath is rapid) it is $\frac{\partial \rho}{\partial p}\big|_T$. Stratification can stabilize against either (or both) of Rayleigh-Taylor or Kelvin-Helmholtz instabilities.

This criterion ignores the stabilizing effect of viscosity, which is small at high Reynolds numbers and not easy to calculate when both shear and stratification affect stability. At lower Reynolds numbers (defined by zone size), viscosity is significant but calculated directly by a hydrodynamics code. When this is the case subgrid scale turbulence does not occur and, provided the Schmidt number is $\mathcal{O}(1)$ molecular diffusivity is rapid and no turbulent diffusivity model is required.

The factor of $1/6$ is introduced to allow for three spatial dimensions (in analogy with the factor $1/3$ in the elementary kinetic theory result $D = u\ell/3$, where ℓ is the mean free path), and for the double counting resulting from symmetrization of e_{ij} . Because the proposed form is phenomenological, if fitting data are available it may be appropriate to introduce an additional dimensionless multiplicative factor chosen to match those data. Such “data” may be obtained from a fine scale but idealized 3-D numerical hydrodynamic calculation of turbulent mix, for example in an unstratified isochoric (constant and uniform density) fluid.

When this model is applied to an Eulerian calculation it is tacitly assumed that an interface-preserving algorithm is used to prevent rapid numerical diffusion of composition that may be entirely spurious (for example, if the stratification is stable).

V. DISCUSSION

Turbulent mixing is a problem of long standing, and many models have been introduced. Typically they involve several free parameters, and these may be chosen to give excellent fits in regions of parameter space for which appropriate data are available. For example, the widely used BHR model[3, 20] contains ten fitting parameters. These have been chosen to fit a classic shock tube experiment[21]. With so many parameters available the fit is excellent, but that does not establish its validity when extrapolated outside the range of conditions to which they were fitted. For many important problems no data exist in the parameter range of interest. A simple model may be more robust than a sophisticated one.

Any model, and especially one as oversimplified as that proposed here, needs to be tested. Quantitative experimental tests are few because of the difficulty of measuring (and even defining in an experimentally accessible manner) effective diffusion coefficients for complex heterogeneous flows. Numerical simulation may be a preferable approach, because there is no difficulty in defining spatial distributions of composition, and even of fitting an effective D to the evolution of their means. An unstable velocity field is set up on a fine mesh, and the mixing calculated by the code is compared to that produced by the model applied to a much coarser description of the mean velocity field. Both the validity of the model and the optimal value of any multiplicative coefficient may be determined from this comparison.

Subgrid turbulent viscosity and heat transport present problems analogous to that of subgrid turbulent mixing. Sophisticated models exist, but also contain several parameters (essentially closure parameters for the moment equations). It may be a reasonable rough approximation to use the model proposed here for D_{turb} and to take $\nu_{turb} = Sc_{turb}D_{turb}$, estimating Sc_{turb} from numerical simulations like those used to test the model for D_{turb} , or simply taking $\nu_{turb} = D_{turb}$ in the absence of such information. Similarly, it may be reasonable to take $\alpha_{turb} = D_{turb}$.

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